

## Chemical Safety Data Sheet MSDS / SDS

**2-Benzyl-3-oxo-2,3-dihydro-1H-isoindole-4-carboxylic acid**

Revision Date:2026-09-13 Revision Number:1

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****Product identifier**

Product name : 2-Benzyl-3-oxo-2,3-dihydro-1H-isoindole-4-carboxylic acid  
CBnumber : CB5392902  
CAS : 77960-29-3  
Synonyms : 2-benzyl-3-oxoisindoline-4-carboxylic acid; 1H-Isoindole-4-carboxylic acid, 2,3-dihydro-3-oxo-2-(phenylmethyl)-

**Relevant identified uses of the substance or mixture and uses advised against**

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

**Company Identification**

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 010-86108875

**SECTION 2: Hazards identification****GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

**Precautionary statements**

P264 Wash skin thoroughly after handling.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P332+P313 IF SKIN irritation occurs: Get medical advice/attention.  
P337+P313 IF eye irritation persists: Get medical advice/attention.

**Hazard statements**

H315 Causes skin irritation  
H319 Causes serious eye irritation

**SECTION 3: Composition/information on ingredients**

## Substance

|              |                                                                                                                   |
|--------------|-------------------------------------------------------------------------------------------------------------------|
| Product name | : 2-Benzyl-3-oxo-2,3-dihydro-1H-isoindole-4-carboxylic acid                                                       |
| Synonyms     | : 2-benzyl-3-oxoisindoline-4-carboxylic acid; 1H-Isoindole-4-carboxylic acid, 2,3-dihydro-3-oxo-2-(phenylmethyl)- |
| CAS          | : 77960-29-3                                                                                                      |
| MF           | : C <sub>16</sub> H <sub>13</sub> NO <sub>3</sub>                                                                 |
| MW           | : 267.28                                                                                                          |

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air.

#### In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

#### If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

### 4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11

### 4.3 Indication of any immediate medical attention and special treatment needed

No data available

### 4.4 Notes to physician

No data available

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

#### Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Combustible.

Development of hazardous combustion gases or vapours possible in the event of fire.

### 5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact.

Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

### 6.2 Environmental precautions

Do not let product enter drains.

### 6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

### 6.4 Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

For precautions see section 2.2.

### 7.2 Conditions for safe storage, including any incompatibilities

#### Storage conditions

Tightly closed. Dry.

#### Storage class

Storage class (TRGS 510): 11: Combustible Solids

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

## 8.2 Exposure controls

### Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

### Personal protective equipment

#### Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

#### Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-

approved gloves (e.g. KCL GmbH, D-36124 Eichenzell,

Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 L

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 L

### Body Protection

protective clothing

### Respiratory protection

required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

### Control of environmental exposure

Do not let product enter drains.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

|                                            |                          |
|--------------------------------------------|--------------------------|
| a) Physical state                          | solid                    |
| b) Color                                   | No data available        |
| c) Odor                                    | No data available        |
| d) Melting point/freezing point            | No data available        |
| e) Initial boiling point and boiling range | 530.3±50.0 °C(Predicted) |
| f) Flammability (solid, gas)               | No data available        |

g) Upper/lower flammability or explosive limits No data available

limits

|                                          |                                                                                  |
|------------------------------------------|----------------------------------------------------------------------------------|
| h) Flash point                           | Not applicable                                                                   |
| i) Autoignition temperature              | No data available                                                                |
| j) Decomposition temperature             | No data available                                                                |
| k) pH                                    | No data available                                                                |
| l) Viscosity                             | Viscosity, kinematic: No data available<br>Viscosity, dynamic: No data available |
| m) Water solubility                      | at 25 °C soluble                                                                 |
| n) Partition coefficient n-octanol/water | log Pow: 1.04 at 25 °C - Bioaccumulation is not expected.                        |
| o) Vapor pressure                        | No data available                                                                |
| p) Density                               | 1.357±0.06 g/cm <sup>3</sup> (Predicted)                                         |
| Relative density                         | 1.357±0.06 g/cm <sup>3</sup> (Predicted)                                         |
| q) Relative vapor density                | No data available                                                                |
| r) Particle characteristics              | No data available                                                                |
| s) Explosive properties                  | Not classified as explosive.                                                     |
| t) Oxidizing properties                  | No data available                                                                |

## 9.2 Other safety information

No data available

# SECTION 10: Stability and reactivity

## 10.1 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

## 10.2 Possibility of hazardous reactions

No data available

## 10.3 Conditions to avoid

no information available

## 10.4 Incompatible materials

Strong oxidizing agents

## 10.5 Hazardous decomposition products

In the event of fire: see section 5

# SECTION 11: Toxicological information

## 11.1 Information on toxicological effects

### Acute toxicity

Oral: No data available

Inhalation: No data available

Dermal: No data available

#### **Skin corrosion/irritation**

Remarks: The value / statement given is based on a (Q)SAR approach

#### **Serious eye damage/eye irritation**

Remarks: The value / statement given is based on a (Q)SAR approach

#### **Respiratory or skin sensitization**

Classified based on available data. For more details, see section 2

#### **Germ cell mutagenicity**

Test Type: Chromosome aberration test in vitro

Method: QSAR

Result: positive

Remarks: The value / statement given is based on a (Q)SAR approach

Test Type: Micronucleus test

Method: QSAR

Result: positive

Remarks: The value / statement given is based on a (Q)SAR approach

Test Type: comet assay

Method: QSAR

Result: positive

Remarks: The value / statement given is based on a (Q)SAR approach

#### **Carcinogenicity**

Potential cancer hazard.

#### **Reproductive toxicity**

Classified based on available data. For more details, see section 2

#### **Specific target organ toxicity - single exposure**

Classified based on available data. For more details, see section 2

#### **Specific target organ toxicity - repeated exposure**

Classified based on available data. For more details, see section 2

#### **Aspiration hazard**

Classified based on available data. For more details, see section 2

### **11.2 Additional Information**

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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## **SECTION 12: Ecological information**

### **12.1 Toxicity**

No data available

### **12.2 Persistence and degradability**

Biodegradability

Result: - Not readily biodegradable.

Remarks: The value / statement given is based on a (Q)SAR approach

### **12.3 Bioaccumulative potential**

No data available

### **12.4 Mobility in soil**

No data available

### **12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

### **12.6 Endocrine disrupting properties**

No data available

### **12.7 Other adverse effects**

No data available

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## **SECTION 13: Disposal considerations**

### **13.1 Waste treatment methods**

Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

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## **SECTION 14: Transport information**

### **14.1 UN number**

ADR/RID: -

IMDG: -

IATA-DGR: -

### **14.2 UN proper shipping name**

ADR/RID: Not dangerous goods

IMDG: Not dangerous goods

IATA-DGR: Not dangerous goods

### **14.3 Transport hazard class(es)**

ADR/RID: -

IMDG: -

IATA-DGR: -

### **14.4 Packaging group**

ADR/RID: -

IMDG: -

IATA-DGR: -

#### **14.5 Environmental hazards**

ADR/RID: no

IMDG Marine pollutant: no

IATA-DGR: no

#### **14.6 Special precautions for user**

#### **14.7 Incompatible materials**

Strong oxidizing agents

Further information: Not classified as dangerous in the meaning of transport regulations.

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## **SECTION 15: Regulatory information**

### **15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**

National regulatory information

Measures on the Environmental Administration of New Chemical Substances Registration

Registration/Notification number : B1A222223087

Downstream users need to comply with the conditions of safe use of the chemical, understand the environmental and health hazard and risk management measures identified on the SDS as well as the local/national regulations concerning the chemical.

Other regulations

Please pay attention on the waste treatment should also comply with local regulations requirement.

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## **SECTION 16: Other information**

### **Abbreviations and acronyms**

CAS: Chemical Abstracts Service

TWA: Time-Weighted Average

STEL: Short-Term Exposure Limit

LD50: Lethal Dose 50%

LC50: Lethal Concentration 50%

EC50: Effective Concentration 50%

PEL: Permissible Exposure Limit

TLV: Threshold Limit Value

IMDG: International Maritime Dangerous Goods Code

IATA: International Air Transport Association

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

DOT: US Department of Transportation

NFPA: National Fire Protection Association

NIOSH: National Institute for Occupational Safety and Health

OSHA: Occupational Safety and Health Administration

**Disclaimer:**

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.